

1-D Dirac equation, Klein Paradox and Graphene

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Abstract

Solutions of the one dimensional Dirac equation with piece-wise constant potentials are presented following standard methods. These solutions show that the Klein Paradox is non-existent and represents a failure to correctly match solutions across a step potential. Consequences of this exact solution are studied for the step potential and a square barrier. Characteristics of massless Dirac states and the momentum linear band energies for Graphene are shown to have quite different current and momentum properties.

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I. INTRODUCTION

The renewed interest in graphene[1] and the close analogy of its band structure to the spectrum of the zero mass Dirac equation suggests that a re-examination of several aspects of the one dimensional Dirac equation should be carried out. The first of these aspects is the well known Klein paradox[2] which continues to persist in the literature. The second of these aspects is the question of how closely the graphene spectrum resembles the Dirac spectral properties and states. Dragoman in an excellent paper[3] has recently examined some of these issues and has noted that there is no Klein Paradox. In this paper we will examine the mathematics of solutions to the one dimensional Dirac equation in the presence of a piece-wise constant potential step (the Klein problem). The solutions of this differential equation are exact and can be carried out analytically. The usual method of analysis will involve the delta function normalization of wave functions in the continuous spectrum. In order to clarify some of the mathematical details a slightly more meticulous method of calculation originally suggested by Von Neumann[4] will be followed so that all of the mathematical inferences can be carried out transparently. In the first section details of the solutions of the differential equation will be discussed. At the end of that section the wave function solutions for the potential step will be exhibited. This will show that the Klein paradox arises because of a mis-application of the solutions of piece-wise constant potentials for these one dimensional Dirac equations. In the next section will be a short discussion of the admixture of free negative energy states into the positive energy states for this step potential system if the potential were to be turned on instantaneously. This admixture should monitor the creation of electron-positron pairs near the potential step. After this admixture discussion a characteristic of orthogonality in the thermodynamic limit will be discussed. The reflection coefficient for finite width square potential barriers will be displayed and finally the effect of piece-wise constant potential steps on zero mass states will be discussed as well as a comparison with both the energy spectrum and current densities for a "one dimensional" Graphene.

II. SOLUTIONS OF PIECE-WISE CONSTANT POTENTIAL DIFFERENTIAL EQUATIONS

One dimensional solutions of the Schrodinger and Dirac equations essentially reduce to finding the finite, continuous, and differentiable solutions of a Sturm-Liouville type of differential equation on the whole line interval $(-\infty, \infty)$ [5],[7]. For the discrete spectrum of such equations there is an orthonormal set of eigenstates. For the continuous spectrum the momentum eigenstates are functions that can only be normalized with Dirac delta functions. The delta function normalization is generally quite satisfactory except for some calculations involving squares of delta functions.

Because of a desire to be mathematically careful and transparent in this examination of the Klein paradox, a procedure will here be followed that dates back to von Neumann[4] and many others[6]. Specifically, all of the wave functions to be used here will be "box normalized" in regions of length L and final results will be obtained in the thermodynamic limit ($L \rightarrow \infty$). Within the interval of length L the allowed momentum values will be discrete $k = 2\pi n/L$, where n is an integer. This whole process will not be essential for the demonstration that the Klein paradox is not a paradox at all, but will be useful in studying the admixture of free particle states and those interacting states in the presence of the potential step. For each finite L we will find that the eigenvalue spectrum will be discrete and that in the thermodynamic limit ($L \rightarrow \infty$) the spectrum becomes continuous and the eigenstates become delta function normalized. Details of the transition to the thermodynamic limit have been discussed in detail by Messiah[7], Arfken and Weber[8], and Sneddon[9] and some of these details will be discussed in the following.

The Dirac equation with a constant potential has exact solutions which are the same as the free particle solutions except that the energy E_k can be different from the free particle case

$$E_k = V_0 \pm \sqrt{m^2 + k^2} \quad (1)$$

by the addition of the constant potential. In order to simplify the notation in this study the velocity of light $c = \hbar = 1$ will be used in the formulas to follow. The Dirac equation will be studied with 2×1 spinors for simplicity. This is a standard simplification sometimes described as "no spin" or "single spin". The basic idea of this paper is that we consider these solutions to Dirac equations in two regions $(-L, 0)$ and $(0, L)$ and construct all wave

functions out of two parts

$$\Psi(z) = \psi_L(z)\Theta(-z) + \psi_R(z)\Theta(z) \quad (2)$$

where $\Theta(z)$ is the Heaviside function (unit step function at zero), $\psi_L(z)$ is a solution in the left side interval $(-L, 0)$ and $\psi_R(z)$ is a solution in the right interval $(0, L)$. The boundary condition is that the two solutions be continuous at the origin

$$\psi_L(0^-) = \psi_R(0^+). \quad (3)$$

In each region, $(-L, 0)$ and $(0, L)$, the orthonormal positive and negative energy states, respectively, are given by

$$p_k(z) = \frac{1}{\sqrt{L}} \frac{1}{\sqrt{1+u_k^2}} \begin{pmatrix} 1 \\ u_k \end{pmatrix} e^{ikz} \quad (4)$$

and

$$n_{-k}(z) = \frac{1}{\sqrt{L}} \frac{1}{\sqrt{1+u_k^2}} \begin{pmatrix} u_k \\ 1 \end{pmatrix} e^{-ikz} \quad (5)$$

where

$$u_k = \frac{k}{m + \sqrt{m^2 + k^2}}. \quad (6)$$

Both of the orthonormal solutions above are written for a positive-direction probability current density J_k which is given by

$$J_k = \frac{2u_k}{1+u_k^2}. \quad (7)$$

Reversing the k value gives the current in the negative direction carrying states. The energies of these states will depend on the side of the origin. On the left the energy will be $\pm\sqrt{m^2 + k^2}$ and on the right $V_0 \pm \sqrt{m^2 + k'^2}$. In the following paragraphs the wave vectors on the right side ($z \geq 0$) will be indicated with a prime as k' .

On either side of the origin these solutions are orthonormal

$$\langle n_k | n_{k'} \rangle = \langle p_k | p_{k'} \rangle = \Delta_{k,k'} = \frac{e^{i(k-k')L} - 1}{i(k - k')L} \quad (8)$$

where $\Delta_{k,k'}$ is the Kronecker delta, $\Delta_{k,k'} = 1$ if $k - k'$ and zero if $(k - k')L = 2\pi(n - n') \neq 0$. In each interval the allowed momentum values are $k = 2\pi n/L$, where n is any integer. Similarly, $\langle n_k | p_{k'} \rangle = 0$. The discrete k values are those which guarantee that the momentum operator

is hermitian, namely, that $\psi^\dagger(0)\psi(0) = \psi^\dagger(L)\psi(L)$ for the right side, and similarly on the left side. The usual delta function nromalization is achieved by removing the normalization factor $1/\sqrt{L}$ from each wave function and recalling that for all sequences leading to the thermodynamic limit

$$\lim_{L \rightarrow \infty} L\Delta_{k,k'} = \delta(k - k') \quad (9)$$

where $\delta(k - k')$ is the Dirac delta function. In the following it will often be the case that the normalizations for each half interval $1/(\sqrt{L}\sqrt{1+u_k^2})$ will be discarded and normalization on the whole interval $(-L, L)$ will be re-calculated.

For the Dirac equation on the whole interval $(-\infty, \infty)$ there are no states in the mass gap $-m \leq E \leq m$. But, for each of the two half intervals there are evanescent (exponential) wave functions that preserve momentum hermiticity. These are labeled by a complex momentum $i\kappa$ and have both positive and negative energy relative to the center of the mass gap $V_0 \pm \sqrt{m^2 - \kappa^2}$ and can be written for each fixed L in the sequence as

$$O_\kappa^{(>+)}(z) = \begin{pmatrix} 1 \\ iw_\kappa \end{pmatrix} e^{-\kappa z} + e^{-\kappa L} \begin{pmatrix} 1 \\ -iw_\kappa \end{pmatrix} e^{\kappa z} \quad (10)$$

$$O_\kappa^{(>-)}(z) = \begin{pmatrix} -iw_\kappa \\ 1 \end{pmatrix} e^{-\kappa z} + e^{-\kappa L} \begin{pmatrix} iw_\kappa \\ 1 \end{pmatrix} e^{\kappa z} \quad (11)$$

where

$$w_\kappa = \frac{\kappa}{m + \sqrt{m^2 - \kappa^2}}, \quad (12)$$

for the interval $(0, L)$. Similar functions $O_\kappa^{(<+)}(z)$ and $O_\kappa^{(<-)}(z)$ are defined for the interval $(-L, 0)$. In the thermodynamic limit the second term vanishes and these functions yield the usual single exponential function.

When the step potential V_0 is zero, there are no allowed states in the mass gap. Even when $0 \leq V_0 \leq 2m$ there are no states in the part of the gap which remains on both sides of the origin.

The general solution is now achieved by equating at the origin the two functions, one from each side at the origin, that have the same energy, and using this equality of energy to determine the relationship between the momenta on the two sides. In Tables (1 and 2) are shown the energy ranges and the structure of the wave functions in each region which have the same energy. Note that for simplicity, we are examining states that initiate

with a current from the left and contain a reflected wave on the left and transmitted wave on the right.

There are two distinct V_0 energy ranges and to simplify the discussion Table 1 shows the wave function pairings and the relationships between the left and right side momenta for small $0 \leq V_0 \leq 2m$ and Table 2 shows the same for $V_0 > 2m$. The table shows the wave functions and the relationship between the momenta on each side of the origin and for each energy range.

Referring to Table I, for small V_0 ($0 \leq V_0 \leq 2m$), we will discuss the states from the top of the Table (highest energy) to the bottom (lowest energy). At the top are the states for which $E_k > V_0 + m$. As can be seen in the Table we have "positive energy" functions $p_k(z) + f_k p_{-k}(z)$ on the left (f_k is the reflection amplitude) and on the right we have $g_k p_{k'}(z)$ where g_k is the transmission amplitude. The next set of functions are in the energy interval $m \leq E_k \leq V_0 + m$, which are of the form $p_k(z) + e^{i\phi} p_{-k}(z)$ in the left side and are matched with an evanescent wave $O_\kappa(z)$ on the right side. Because the evanescent states carry no current, the reflection amplitude has unit magnitude and thus gives complete reflection. The next energy range $V_0 - m \leq E \leq m$ corresponds to the empty mass gap with no wave functions satisfying the boundary condition. The next lower energy range $-m \leq E_{k'} \leq V_0 - m$ corresponds to another combination of which half is evanescent and cannot carry any current. These states have an evanescent wave $O_{-\kappa}(z)$ on the left and $n_k(z) + e^{i\phi} n_{-k}(z)$ on the right. The reflection amplitude again has magnitude 1 as found before for a combination of traveling and evanescent waves. The lowest energy states are the fully negative energy states and have $n_{-k}(z) + f_k n_k(z)$ on the left and $g_k n_{-k'}(z)$ on the right.

As the potential step size V_0 increases and enters into the range $V_0 \geq 2m$, a new pairing of functions that Klein did not consider begins to appear. These states are discussed Table 2. Examining the top of Table 2, the highest energy range $E_k > V_0 + m$ is unchanged from the previous discussion. The second energy range is now expanded to $V_0 - m \leq E_\kappa \leq V_0 + m$ and remains, as before, with complete reflection. The new range $m \leq E_k \leq V_0 - m$ pairs wave functions $p_k(z) + f_k p_{-k}(z)$ on the left with transmitted functions $g_k n_{-k'}(z)$ on the right. The remaining lower energy ranges and functions are not changed significantly from the previous discussion. This new set of solutions on both sides in the energy range $m \leq E_k \leq V_0 - m$ is what Klein did not consider. In the following we will solve for

the reflection and transmission amplitudes for those cases with non-zero probability current density.

For energies above the step, $E_k \geq V_0 + m$ it is straightforward to show that

$$\sqrt{m^2 + k^2} = V_0 + \sqrt{m^2 + k'^2} \quad (13)$$

$$f_k = \frac{(u_k - u'_k)}{(u_k + u'_k)}, \quad g_k = \frac{2u_k}{(u_k + u'_k)}, \quad (14)$$

where

$$u_k = \frac{k}{m + \sqrt{m^2 + k^2}} \quad (15)$$

and

$$u'_k = \sqrt{\frac{\sqrt{m^2 + k^2} - V_0 - m}{\sqrt{m^2 + k^2} - V_0 + m}}. \quad (16)$$

Using the usual definitions of current density, it is easy to determine that the reflection coefficient R and the transmission coefficient T are given by

$$R = |f_k|^2 = \frac{(u_k - u'_k)^2}{(u_k + u'_k)^2} \quad (17)$$

and

$$T = \frac{u'_k}{u_k} g_k^2 = \frac{4u_k u'_k}{(u_k + u'_k)^2} \quad (18)$$

from which it is easy to see that $R + T = 1$.

For the ranges of energies in which the waves on the right (or the left) are evanescent, we easily find that $T = 0$ and $R = 1$.

For the case which Klein did not consider, when $V_0 \geq 2m$ similar calculations yield

$$\sqrt{m^2 + k^2} = V_0 - \sqrt{m^2 + k'^2} \quad (19)$$

$$f_k = \frac{(u_k u'_k - 1)}{(u_k u'_k + 1)}, \quad g_k = \frac{2u_k}{(u_k u'_k + 1)} \quad (20)$$

$$u'_k = \sqrt{\frac{V_0 - \sqrt{m^2 + k^2} - m}{V_0 - \sqrt{m^2 + k^2} + m}}. \quad (21)$$

and u_k is defined as before. The reflection and transmission coefficients are:

$$R = |f_k|^2 = \frac{(u_k u'_k - 1)^2}{(u_k u'_k + 1)^2} \quad (22)$$

and

$$T = \frac{u'_k}{u_k} g_k^2 = \frac{4u_k u'_k}{(u_k u'_k + 1)^2} \quad (23)$$

from which it is also easy to see that $R + T = 1$.

From these calculations it is clear that there is no paradox. Klein simply did not match the appropriate solutions in the two regions. This mis-match is what is responsible for the usual assumption of a failure of particle conservation (usually taken to imply the production of particle hole pairs near the potential step) that has been so often interpreted as the meaning of the Klein paradox. These analytic solutions show that particle number is always conserved independent of the size of the step potential. The surprising phenomena is that the barrier is close to being transparent in a certain energy range if the step height V_0 is large enough. This behavior of the reflection coefficient is shown in Fig. 1 where the reflection coefficient R has been simultaneously plotted for three different values of $V_0 = 0.5m, 3m, 8m$. In all of these cases there is a region of complete reflection with an energy width of $2m$ and centered on the value of V_0 . At higher energies the reflection coefficient decreases with increasing energy.

The surprising result is that the reflection coefficient decreases in the energy interval $m \leq E_k \leq V_0 - m$ and the barrier becomes partially transparent in this energy range. This result is an exact consequence of the matching of exact solutions in the two regions joined by the boundary condition. On physical grounds this result would seem to be unexpected, but the potential step has pulled what used to be negative energy states into a positive energy range and their ability to carry current leads to the partial transparency of the potential step in this energy range. One possible origin for this surprising phenomena could be with Dirac's original choice for adding potential energies onto the free particle Dirac Hamiltonian.

III. OVERLAP BETWEEN STATES OF NON-INTERACTING AND INTERACTING HAMILTONIANS

Another aspect of the behavior of this system can be probed by studying the overlap of these interacting states in the presence of the potential step with the free states of the free particle Hamiltonian. This is equivalent to asking how the wave functions are matched in the sudden approximation if the step potential were instantaneously turned on. If there were a production of extra electron positron pairs by the potential step, it could be expected

that this overlap would be an indicator of such when the potential V_0 becomes larger than $2m$. In order to carry out this estimate we would need to calculate

$$N = \sum_{k'', P_k} |\langle n_{k''} | P_k \rangle|^2, \quad (24)$$

where $n_{k''}(z)$ is a negative energy wave function of the zero potential Hamiltonian spanning both intervals $(-L, 0)$ and $(0, L)$, and $P_k(z)$ represents any positive energy state of the Hamiltonian with the potential step V_0 . And the expression is summed over all positive energy states with non-zero matrix elements.

It is first important to notice that all of the positive energy states of on both sides of the potential step, which are above the mass gaps on each side, will have no contribution to this matrix element because all of these states are made up of linear combinations of $p_k(z)$ and $p_{-k}(z)$ which are orthogonal to $n_{k''}(z)$ in both of the intervals $(-L, 0)$ and $(0, L)$. So, the only states that can overlap with the negative energy states can be:

- (1) evanescent states in the mass gaps (which will be shown to be negligible in the thermodynamic limit, see Appendix I),
- (2) the negative energy states $n_k(z) + e^{i\phi} n_{-k}(z)$ in the range $-m \leq E_{k'} \leq V_0 - m$ which are matched with evanescent states. The wave functions for these are of the form

$$\Psi_2(z) = A_2((O_{-\kappa}(z)\Theta(-z) + (n_{k'}(z) + e^{i\phi} n_{-k'}(z))\Theta(z)), \quad (25)$$

and

- (3) positive energy states appearing when $V_0 \geq 2m$ which carry current on both sides

$$\Psi_3(z) = A_3((p_k(z) + f_k p_{-k}(z))\Theta(-z) + (g_k n_{-k'}(z))\Theta(z)). \quad (26)$$

Before evaluating these three cases, it is possible to arrive at an intuitive estimate of this quantity by simply asking from a density of states perspective how many of these originally negative energy states have been pulled up from energy $-m$ to positive energies $V_0 - \sqrt{m^2 + k^2}$ by the magnitude of V_0 . If we ignore the boundary conditions, the number of such states would be given by the integral

$$\frac{L}{2\pi} \int_0^{\sqrt{V_0(V_0+2m)}} dk = \frac{L\sqrt{V_0(V_0+2m)}}{2\pi}. \quad (27)$$

Let us first examine case (2). The first step is to evaluate the normalization A_2 which yields

$$A_2(k) = \frac{1}{\sqrt{L(2(1 + u_{k'}^2) + \frac{(1-e^{-\kappa L})}{\kappa L})}}. \quad (28)$$

Neglecting terms of order $1/L$ and smaller and using the orthogonality of $n_{k'}(z)$ and $n_{k''}(z)$ it is straightforward to show that

$$\langle n_{k''} | \Psi_2(k) \rangle = \frac{1}{2} (\Delta_{k'',k'} + e^{i\phi} \Delta_{k'',-k'}). \quad (29)$$

Now, for each L in the sequence to the thermodynamic limit, it is true that

$$\Delta_{k'',k'}^2 = \Delta_{k'',k'} \quad (30)$$

so we obtain

$$|\langle n_{k''} | \Psi_2(k) \rangle|^2 = \frac{1}{4} (\Delta_{k'',k'} + \Delta_{k'',-k'}). \quad (31)$$

This implies that

$$N_2 = \sum_{k'',k} |\langle n_{k''} | \Psi_2(k) \rangle|^2 = \frac{1}{2} \sum_{k'} 1 = \frac{L}{4\pi} \sqrt{V_0(V_0 + 2m)} \quad (32)$$

for the energy range $-m \leq E_{k'} \leq V_0 - m$. If $V_0 > 2m$, the lower limit of the k' integration becomes $\sqrt{V_0(V_0 - 2m)}$ so that the expression for N_2 in that case becomes

$$N_2 = \frac{L}{4\pi} (\sqrt{V_0(V_0 + 2m)} - \sqrt{V_0(V_0 - 2m)}). \quad (33)$$

Now let us examine case (3). In this case the matrix element becomes

$$\langle n_{k''} | \Psi_3(k) \rangle = A_3(k) g_k \int_0^L n_{k''}(z)^\dagger n_{-k'}(z) dz \quad (34)$$

where

$$A_3(k) = \frac{1}{\sqrt{(1+u_k^2)(1+f_k^2) + g_k^2(1+u_{k'}^2)}}. \quad (35)$$

Substituting for f_k^2 and g_k from the eqn. (20) and (21) above, we find

$$\langle n_{k''} | \Psi_3(k) \rangle = \frac{\sqrt{2}u_k \sqrt{(1+u_{k'}^2)} \Delta_{k'',-k'}}{\sqrt{u_k^2 u_{k'}^2 (3+u_k^2) + (1+3u_k^2)}}. \quad (36)$$

So, the contribution from this case is

$$N_3 = \frac{L}{2\pi} \int_0^{\sqrt{V_0(V_0-2m)}} \frac{2u_k^2(1+u_{k'}^2)}{u_k^2 u_{k'}^2 (3+u_k^2) + (1+3u_k^2)} dk. \quad (37)$$

The remaining case 1 is analyzed in Appendix I and gives a result which is not extensive with the length L and so makes no contribution in the thermodynamic limit. The details

and certain aspects of orthogonality in the thermodynamic limit are presented in Appendix I.

The dependence of N on the barrier height V_0 is shown in Fig. 2. For small V_0 the intuitive estimate and the exact result agree. When the potential height becomes greater than $2m$, the lower limit of Eqn. (33) and the integral for N_3 makes their contribution. The smooth curve is the intuitive estimate given by Eqn. (32) and the lower curve with the kink at $V_0 = 2m$ is the exact result for this quantity. Note that the behavior of this quantity is smooth after the threshold $V_0 = 2m$ and less than the intuitive estimate.

IV. TRANSMISSION THROUGH SQUARE BARRIERS

Walker and Gathright[10] worked out all possible one dimensional transfer matrices for the non-relativistic Schrodinger equation across potential discontinuities. They constructed transfer matrices for any arrangement of potential discontinuities by building the transfer matrices out of products of two different matrices: the discontinuity matrix d and the propagation matrix P . All such possible matrices have been worked out for the Dirac equation and will be presented elsewhere. For the one dimensional Dirac equation the discontinuity matrix d is of the form

$$d(a, b) = \begin{bmatrix} a + b & a - b \\ a - b & a + b \end{bmatrix}, \quad (38)$$

and the parameters a and b are replaced by 1 or by u_k or iw_κ or by ratios of these depending on the energy range in the segment between two discontinuities of the potential. The propagation matrix is identical to those found by Walker and Gathright

$$P(\alpha) = \begin{bmatrix} e^\alpha & 0 \\ 0 & e^{-\alpha} \end{bmatrix}. \quad (39)$$

Once relativistic matrices d and P have been constructed for all possible pairs of states which are possible at a discontinuity, it is immediate to construct the transfer matrices that will connect the two solutions at the ends of a region l where the potential has a constant value V_l . A simple, symmetric example of the use of these transfer matrices is a square barrier whose height is $V_0 = 5.5$ and whose width is $a/L = 5/150 = 1/30$. A plot of the reflection coefficient R versus the momentum of the initial wave k is shown in Fig. 3 .

Notice the Ramsauer minima (peaks in T) in the Reflection coefficient.[11] Notice also that the Reflection coefficient for this symmetric case behaves much like the step potential if the potential energy V_0 is larger than the mass gap width and becomes semi-transparent at lower energies.

V. PROPERTIES OF ZERO MASS SOLUTIONS OF THE DIRAC EQUATION

The well known analogy between the band structure of graphene and the energy spectrum of the massless Dirac equation has received much attention recently. For the non-relativistic band structure calculations the velocity of a band state represented by the energy ϵ_k is linear in $|k|$ and is given by $\epsilon_k = \pm v|k|$ (in one dimension). For electronic band structures the current density is proportional to the group velocity which is given by the derivative of the band energies,

$$v_k = \frac{d\epsilon_k}{dk}, \quad (40)$$

and the :"graphene" band structure spectrum will contain both positive and negative velocities for both positive and negative energies (relative to the center of the band).

Examining the zero mass eigenstates of the Dirac equation shows that there are some quite different behaviors than those observed in the non-relativistic band structure for Graphene. The (1+1) Dirac equation has the following simple form in a constant potential V_0

$$\begin{bmatrix} 0 & \frac{d}{dz} \\ \frac{d}{dz} & 0 \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} e^{ikz} = (E - V_0) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} e^{ikz} \quad (41)$$

has eigenstates

$$\Psi_{\pm}(k) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} e^{ikz}. \quad (42)$$

with correspond to the energies

$$E - V_0 = \pm k. \quad (43)$$

The probability current densities carried by these states are:

$$J_+ = \Psi_+^\dagger \sigma_x \Psi_+ = \frac{1}{2} \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 1 \quad (44)$$

and

$$J_- = \Psi_-^\dagger \sigma_x \Psi_- = -1. \quad (45)$$

So the positive direction currents are carried only by positive energies $E - V_0 \geq 0$ and negative direction currents are carried by $E - V_0 \leq 0$. The massless Dirac equation does not allow negative currents to be carried by positive energy eigenstates.

If we consider the reflection at a potential step at $z = 0$ and apply the boundary condition we obtain,

$$k = V_0 + k' \quad (46)$$

and

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} + f_k \begin{pmatrix} 1 \\ -1 \end{pmatrix} = g_{k'} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \quad (47)$$

which yields the equations

$$1 + f_k = g_{k'} \quad (48)$$

$$1 - f_k = g_{k'} \quad (49)$$

which implies that $f_k = 0$ and $g_{k'} = 1$. This condition implies that the potential step makes no reflections for a zero mass particle. This condition and the fact that current direction is so strongly associated with the sign of the energy (relative to V_0) indicates that the analogy between the graphene bandstructure and the massless Dirac equation is not completely accurate.

VI. CONCLUSIONS

The Klein Paradox is not a paradox. It is simply a mis-application of the processes by which the solution of piece-wise constant potential differential equations are constructed. When the appropriate wave functions at the same energies are connected, the reflection and transmission coefficients are continuous functions of the incident wave vector and always obey the conservation of particle number. The surprising characteristic of these solutions is the near transparency of the step potential at low energies if $V_0 > 2m$. This property of the solutions arises from the fact that for large V_0 states which were originally at negative energies are now pulled up into positive energies and it becomes possible for a current to be carried through the step. This result is clearly a property of the solutions of this Dirac equation. The more difficult question is whether this behavior is physically to be expected. This property reflects a choice made by Dirac when he decided to add a potential energy

to his free particle equation. He chose to add it to the $\boldsymbol{\alpha} \cdot \boldsymbol{p}$ as opposed to adding the potential energy to the mass m . These questions have been examined to some extent in other contexts[12].

The connection between the overlap of the negative energy states of the non-interacting Hamiltonian and the Hamiltonian with the potential step, if the latter is turned on instantaneously was examined by studying the summation of the overlap matrix element between positive energy states and the initially negative energy states. It was shown that the accurately determined overlap was consistent with an intuitive picture that the overlap represented the number of negative energy states that have been pulled above the energy $E = -m$. As should be expected because the Klein paradox does not exist, there is no anomalous behavior of this overlap as the potential step is increased above the threshold $V_0 = 2m$.

Generalizing the transfer matrices from the non-relativisitic Schrodinger equation to the Dirac equation allows the treatment of a variety of potential barriers and steps and, numerically, any smooth potential that can be approximated by piece-wise constant potentials in short intervals. By way of an example, the case of a square potential barrier was briefly discussed. The presence of Ramsauer resonances and the transparency of the barrier were found in direct analogy to the results of the step potential.

Finally, zero mass eigenstates of the Dirac equation were examined. Positive current densities were only carried by positive energy states (relative to V_0) and negative current densities were only carried by negative energy states. It appears that a step potential at the origin has no effect on these states. Both of these conditions are quite different from the band structure of Graphene which has stimulated the analogy between that material and the solutions to the Dirac equation. The failure of a step potential to influence the zero energy states seems to be quite unphysical, and seems again to be related to Dirac's original choice by which he added the potential energy to the free particle Dirac equation.

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Surface Weapons Center.

VIII. APPENDIX I: OVERLAP BETWEEN EVANESCENT AND FREE NEGATIVE ENERGY STATES

In this appendix the overlap of the negative energy free particle eigenstates with the evanescent states in the gaps are examined and found to be of order $1/L$.

As an example, consider a state where the overall energy is in the range $V_0 \leq E \leq V_0 + m$. One of the wave functions in this range is

$$\Psi_1(z) = A_1(k)((p_k(z) + e^{i\phi}p_{-k}(z))\Theta(-z) + (g_\kappa e^{-\kappa z} \begin{pmatrix} 1 \\ iw_\kappa \end{pmatrix})\Theta(z)), \quad (\text{A-1})$$

where

$$A_1(k) = \frac{1}{\sqrt{L} \sqrt{2(1+u_k^2) + g_k^2(1+w_\kappa^2) \frac{(1-e^{-2\kappa L})}{\kappa L}}}. \quad (\text{A-2})$$

The matrix element, ignoring terms of order $e^{-\kappa L}$, is

$$\langle n_{k''} | \Psi_1(k) \rangle = \frac{1}{L} \frac{(u_k + iw_\kappa)}{\sqrt{2} \sqrt{(1+u_{k''}^2)} \sqrt{2(1+u_k^2) + \frac{g_k^2}{\kappa L} (1+w_\kappa^2) (\kappa - ik'')}}. \quad (\text{A-3})$$

The contribution of this matrix element to N_1 as $L \rightarrow \infty$ is given by

$$N_1 = \sum_{k'',k} |\langle n_{k''} | \Psi_1 \rangle|^2 = \frac{1}{16\pi^2} \int dk'' \int dk \frac{(u_k^2 + w_\kappa^2)}{(1+u_{k''}^2)(1+u_k^2)(\kappa^2 + k''^2)}. \quad (\text{A-4})$$

Since this integral is not extensive in L when compared to the other contributions which are proportional to L , this contribution is negligible in the thermodynamic limit.

The fact that the overlap of $n_{k''}(z)$ with the evanescent states $O_\kappa(z)$ was negligible in the thermodynamic limit raises a question involving evanescent states in the mass gap and more generally parts of wave functions within the confines of a square potential barrier $0 < z < a < L$. This detail has already been discussed by Arfken and Sneddon in their discussion of the evolution of the fourier integral from the Fourier series in the thermodynamic limit. In their discussion it is observed that in the transition $L \rightarrow \infty$ the constant term $a_0/2$ of the Fourier series becomes negligible in the thermodynamic limit.

Similarly, the corresponding relationship between "box normalized" wave functions in the thermodynamic limit becomes apparent in the theorem for Hermitian operators that

eigenvectors with different eigenvalues must be orthogonal. Consider two states of the type from case 1 with different wave vectors, and thus different energies

$$\Psi_{k_1}(z) = A_1(k_1)((p_{k_1}(z) + e^{i\phi}p_{-k_1}(z))\Theta(-z) + (g_{\kappa_1}e^{-\kappa_1 z} \begin{pmatrix} 1 \\ iw_{\kappa_1} \end{pmatrix})\Theta(z)) \quad (\text{A-5})$$

$$\Psi_{k_2}(z) = A_2(k_2)((p_{k_2}(z) + e^{i\phi}p_{-k_2}(z))\Theta(-z) + (g_{\kappa_2}e^{-\kappa_2 z} \begin{pmatrix} 1 \\ iw_{\kappa_2} \end{pmatrix})\Theta(z)) \quad (\text{A-6})$$

and the energies are:

$$E_{k_1} = \sqrt{m^2 + k_1^2} \neq \sqrt{m^2 + k_2^2} = E_{k_2}. \quad (\text{A-7})$$

If we evaluate the overlap between these two vectors, the integrals on the left hand interval $(-L, 0)$ immediately give zero because of the orthogonality of the p_{k_1} functions. This leaves an integral on the interval $(0, L)$

$$\langle \Psi_{k_1} | \Psi_{k_2} \rangle = A_1 A_2 (0 + \frac{g_{\kappa_1} g_{\kappa_2} (1 + w_{\kappa_1} w_{\kappa_2})}{\sqrt{1 + w_{\kappa_1}^2} \sqrt{1 + w_{\kappa_2}^2} (\kappa_1 + \kappa_2)}). \quad (\text{A-8})$$

On first reflection this second term is not zero and appears to violate the orthogonality theorem, but it must be noted that the factors $A_1 A_2$ provide a factor of $1/L$ and this matrix element vanishes in the thermodynamic limit. The orthogonality of the kind of states combined in the process of joining solutions of piece-wise constant potentials is dominated by the momentum eigenstates and integrals over smaller intervals can be non-zero for finite L , but make no contribution in the thermodynamic limit.

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X. TABLES

Table 1: A tabulation of the energy range and the type of wave functions that are matched at the origin as well as the equation relating the wave vector k on the left and k' on the right for small $V_0 < 2m$. In this example, the two mass gaps have a significant overlap which contains no wave functions.

E range	$\psi_L(z)$	$\psi_R(z)$	k and k'
$E > V_0 + m$	$p_k(z) + f_k p_{-k}(z)$	$g_k p_{k'}(z)$	$\sqrt{m^2 + k^2} = V_0 + \sqrt{m^2 + k'^2}$
$m \leq E \leq V_0 + m$	$p_k(z) + e^{i\phi} p_{-k}(z)$	$g_\kappa O_\kappa(z)$	$\sqrt{m^2 + k^2} = V_0 + \sqrt{m^2 - \kappa^2}$
$V_0 - m \leq E \leq m$	no w.f.	no w.f.	True Mass gap; no states
$-m \leq E \leq V_0 - m$	$g_{-\kappa} O_{-\kappa}(z)$	$n_{k'}(z) + e^{i\phi} n_{-k'}(z)$	$\pm \sqrt{m^2 - \kappa^2} = V_0 - \sqrt{m^2 + k'^2}$
$E \leq -m$	$n_{-k}(z) + f_k n_k(z)$	$g_k n_{-k'}(z)$	$-\sqrt{m^2 + k^2} = V_0 - \sqrt{m^2 + k'^2}$

Table 2: A tabulation of the energy range and the type of wave functions that are matched at the origin as well as the equation relating the wave vector k on the left and k' on the right for large $V_0 > 2m$. The two mass gaps have a significant separation and the function pairs that Klein ignored are included in this energy range.

E range	$\psi_L(z)$	$\psi_R(z)$	k and k'
$E > V_0 + m$	$p_k(z) + f_k p_{-k}(z)$	$g_k p_{k'}(z)$	$\sqrt{m^2 + k^2} = V_0 + \sqrt{m^2 + k'^2}$
$V_0 \leq E \leq V_0 + m$	$p_k(z) + e^{i\phi} p_{-k}(z)$	$g_\kappa O_\kappa^{(+)}(z)$	$\sqrt{m^2 + k^2} = V_0 + \sqrt{m^2 - \kappa^2}$
$V_0 - m \leq E \leq V_0$	$p_k(z) + e^{i\phi} p_{-k}(z)$	$g_\kappa O_\kappa^{(-)}(z)$	$\sqrt{m^2 + k^2} = V_0 - \sqrt{m^2 - \kappa^2}$
$m \leq E \leq V_0 - m$	$p_k(z) + f_k p_{-k}(z)$	$g_k n_{-k'}(z)$	$\sqrt{m^2 + k^2} = V_0 - \sqrt{m^2 + k'^2}$
$0 \leq E \leq m$	$g_{-\kappa} O_{-\kappa}^{(+)}(z)$	$n_{k'}(z) + e^{i\phi} n_{-k'}(z)$	$+\sqrt{m^2 - \kappa^2} = V_0 - \sqrt{m^2 + k'^2}$
$-m \leq E \leq 0$	$g_{-\kappa} O_{-\kappa}^{(-)}(z)$	$n_{k'}(z) + e^{i\phi} n_{-k'}(z)$	$-\sqrt{m^2 - \kappa^2} = V_0 - \sqrt{m^2 + k'^2}$
$E \leq -m$	$n_{-k}(z) + f_k n_k(z)$	$g_k n_{-k'}(z)$	$-\sqrt{m^2 + k^2} = V_0 - \sqrt{m^2 + k'^2}$

XI. FIGURE CAPTIONS

Fig. 1: Three independent plots of the reflection coefficient R versus the wave vector k of the incident wave for three different values of $V_0 = 0.5, 3.0, 8.0$ rest masses are plotted together. Each curve can be identified by the value of k at the center of the $R = 1$ plateau.

Fig. 2: Two curves, one approximate and one exact, for the overlap N between the positive energy states in the presence of the step potential and free negative energy states in the absence of the step potential. The smooth curve is the "intuitive" N derived from the density of negative energy states shifted up by the potential step. The lower curve with the break at $V_0 = 2$ is the complete calculation of N as a function of V_0 for states satisfying the boundary condition. Note that the exact curve does not indicate excessive overlap (electron-positron) pairs above the threshold $V_0 = 2m$.

Fig. 3: A plot of the reflection coefficient R versus the incident wave momentum k for a square barrier with height $V_0 = 5.5$ and width $a/L = 1/30$. Notice the prominent Ramsauer minima.

Figure 1

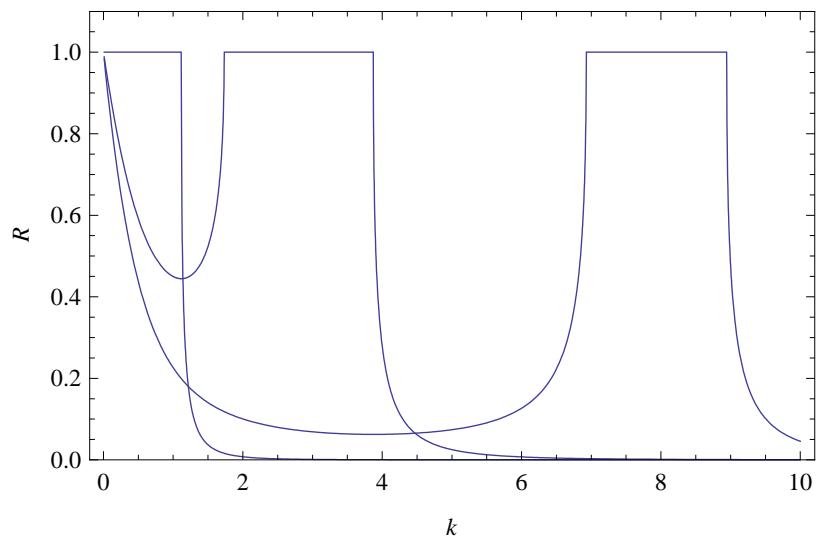


Figure 2

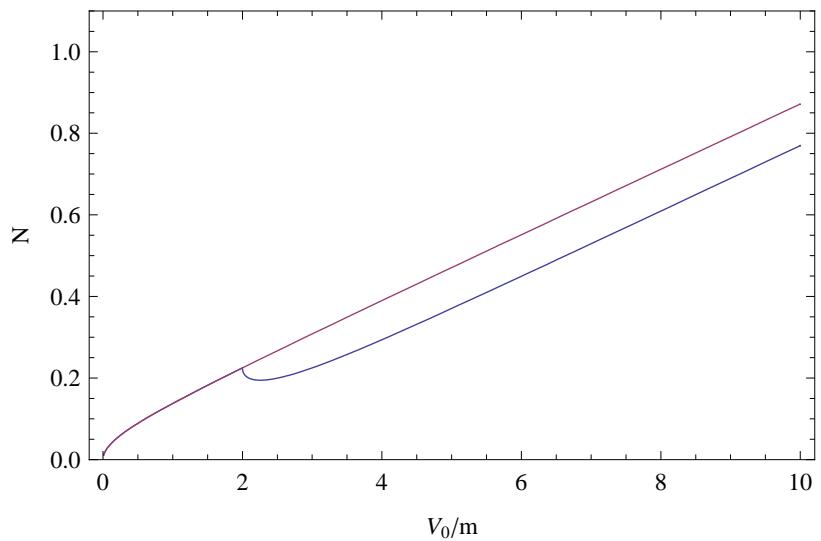


Figure 3

